Overview: ALPS/APEX Plasma Edge & Plasma Material Interaction Modeling Group

Jeffrey N. Brooks

APEX/ALPS meeting, Princeton, Nov. 2002

Plasma Edge and Plasma/Material Interaction Modeling Group

Purpose

Undertake model integration and studies of the plasma edge and plasma/material interactions (PMI) that lead to:

1) fundamental understanding of the influences of plasma facing surfaces on fusion plasma performance

2) identifying performance limits and optimization strategies for advanced liquid and solid, first wall and PFC concepts.

Near Term Goal

Support the ALPS and APEX programs to help determine the feasibility of and optimization strategies for advanced first wall and PFC concepts.

Group Members

J. Brooks (ANL) – Chairman
J-P. Allain (UIUC)
T. Evans (GA)
A. Hassanein (ANL)
S. Krasheninnikov (UCSD)
L. Owen (ORNL)
M. Rensink (LLNL)
T. Rognlien (LLNL)
D. Ruzic (UIUC)
C. Skinner (PPPL)
D. Stotler (PPPL)
R. Maingi (ORNL)
D. Whyte (UW)
C. Wong (GA)

Focus:

- ELM and VDE liquid and solid surface response.

- Lithium PMI science: temp.-dependent sputter yields and energy distribution, Li^+ sputtering and transport/reflection.

- NSTX lithium module PMI analysis.

- Liquid wall erosion/transport/temp. limits

- Carbon and hydrocarbon erosion/transport, MD code reflection calculations, tritium codeposition analysis/cleanup.

- DEGAS code supporting analysis of current tokamaks.

· **Integrated NSTX lithium erosion analysis**

REDEP/WBC sputtering erosion analysis using:

1. UEDGE (Ronglien et al.) near-surface low-recycle plasma parameters: “**high-power case**” and “**low-power case**”
2. Lithium surface temperature (Ulrickson et al.) {*not self-consistent for high-power case*}
3. Surface temperature dependent sputter yields (Allain et al.)
4. Sputtered Li^+ transport model (Brooks, Allain et al.)

· **Sputtered Li^+ transport model**

Issue and 1st-order model defined, detailed work in progress (with UIUC).

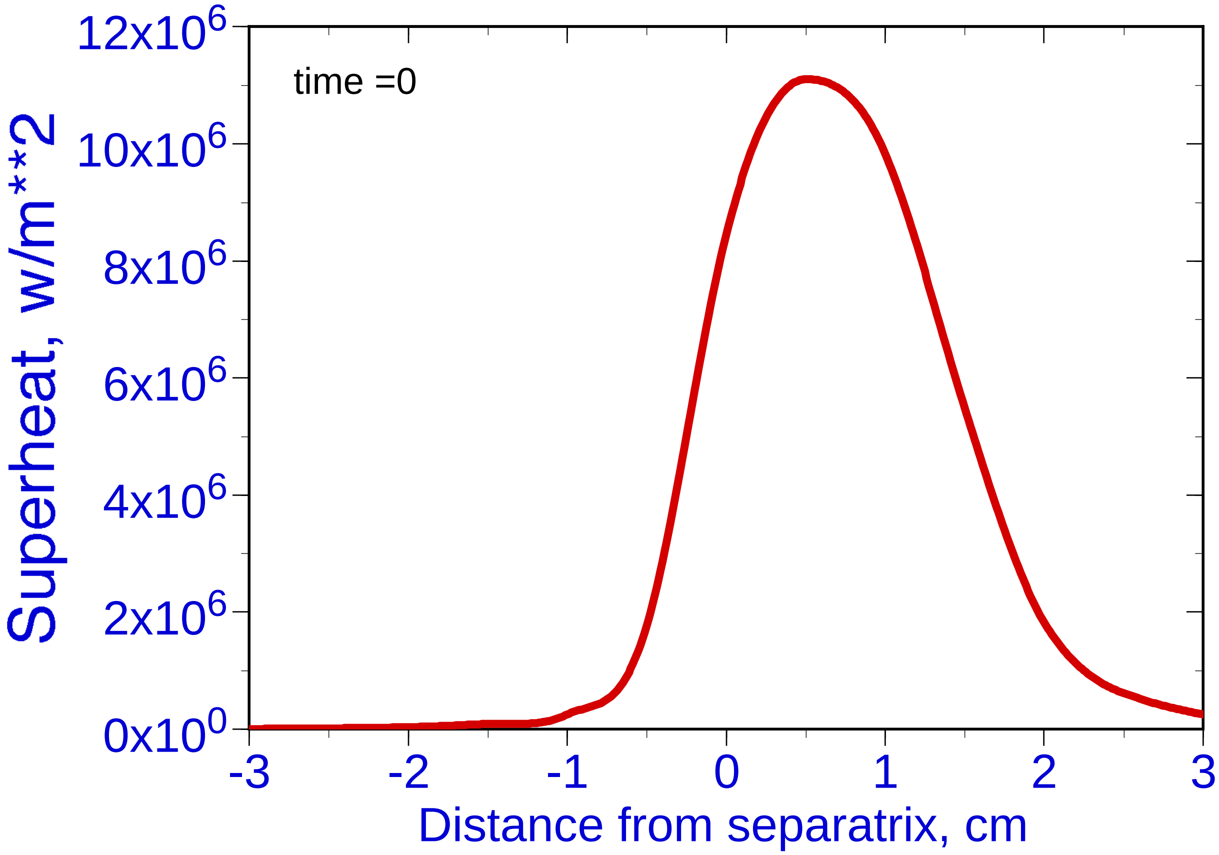
· **WBC/UEDGE coupling**

Code (kinetic/fluid) coupling for complete SOL lithium transport calculations. WBC/UEDGE calibration & test study.

· **Runaway self-sputtering issue**

Self-consistent model (preliminary) developed for sputtered/redeposited lithium superheat, and effect on lithium surface temperature. **Runaway is a concern for high-power case**.

NSTX Lithium Module High-Power Case:
Sputter/redeposition Superheat-WBC analysis



Update on Misc. PSI Issues

J.N. Brooks

- JET: MK-II carbon divertor erosion/co-deposition analysis (ANL, IPP, UIUC, GA, UCSD)—**high T/C codeposition partially explained**.

- FIRE: erosion/redeposition analysis of mixed beryllium/tungsten divertor (ANL, UIUC, LLNL) —**low Be wall erosion.**

- ITER-FEAT: carbon divertor erosion, tritium codeposition estimates (ANL, ITER) — T/C rate **~ 1 mgT/s**

- DiMES Li shots: WBC/MCI analysis (ANL/GA) —**complete SOL Li transport predictions.**

Summary of plasma-surface interaction work at the UIUC

J.P. Allain, D.A. Alman,

M. Nieto, M.D. Coventry,

and D.N. Ruzic

University of Illinois, Urbana-Champaign

Department of Nuclear, Plasma and Radiological Engineering

Plasma-Material Interaction Group

ALPS Meeting, Princeton, New Jersey

November 6-8, 2002

PLASMA MATERIAL INTERACTION GROUP

Outline of Work at the UIUC

- Molecular Dynamics simulations of hydrocarbon plasma-material interaction
- Molecular Dynamics simulations of liquid lithium to study low energy reflection
- Analytical studies of backscattered and sputtered charge fraction at low energies
- FIRE modeling of plasma-material interactions at the first wall and divertor regions
- Liquid metal erosion work in IIAX
- Results of particle retention of free surface flowing liquids in FLIRE (i.e. liquid Li)

PLASMA MATERIAL INTERACTION GROUP

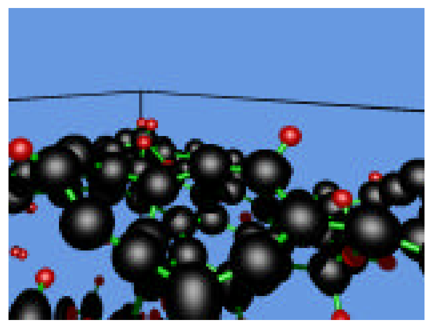
Molecular dynamics modeling of carbon-based surfaces

- Determined reflection coefficients for carbon dimers (C_2) and trimers (C_3)
  - Data, together with previous MolDyn results, used in WBC modeling of DiMES hydrocarbon spectroscopy experiment
- Work is ongoing to extend the hydrocarbon potential to higher energies
  - Brenner potential describes the bonding region of the hydrocarbon potential well
  - The small-separation, repulsive portion is not as good- meaning higher energy collisions are less accurate
  - Higher energy capability is needed for above DiMES modeling, for example, where the plasma temperature is 20 eV

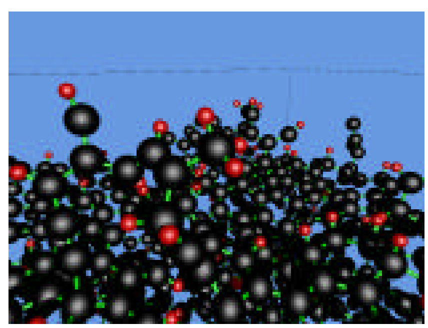
PLASMA MATERIAL INTERACTION GROUP

Carbon-based surfaces used

- Up to now used a hydrogen saturated graphite surface
  - Prepared by bombarding originally pure graphite surface with hydrogen
- Developed a “soft” carbon layer
  - Formed by redeposition of thousands of hydrocarbons on an originally pure graphite surface
- In experiments, these layers tend to be:
  - Polymer-like
  - Less dense
  - Higher H:C ratio
  - Weakly bound → larger sputtering yield



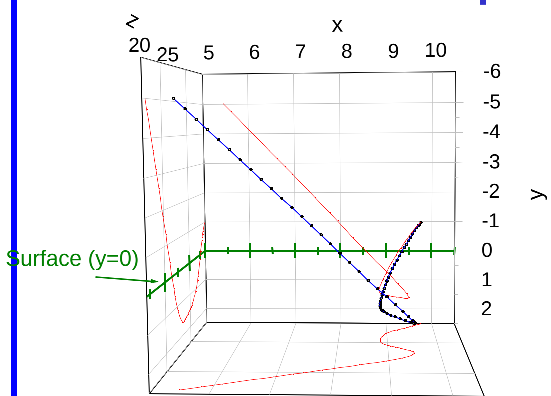
Previous:
H implanted in graphite, result ~0.4 H:C

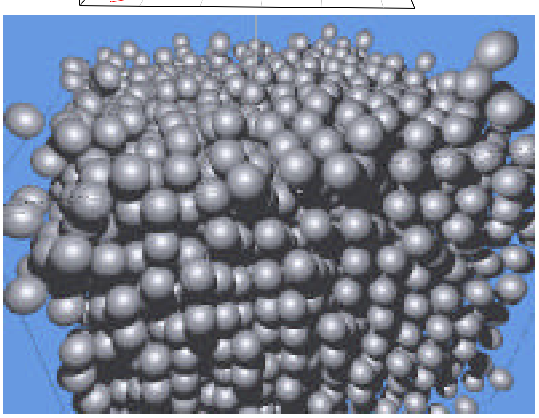


New:
“soft” layer of redeposited hydrocarbons

PLASMA MATERIAL INTERACTION GROUP

MD modeling of lithium bombardment on liquid lithium surfaces



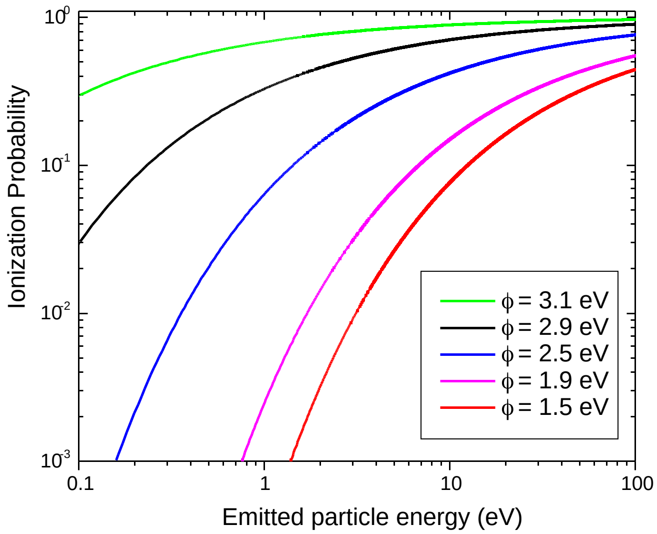


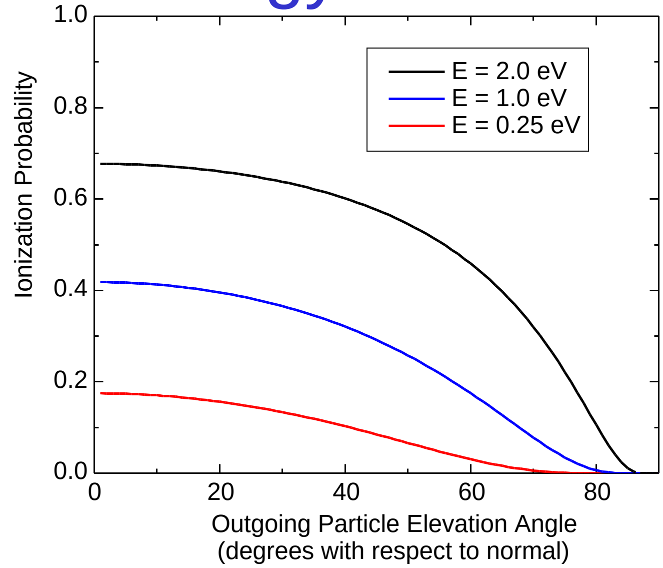
- Preliminary investigation of reflection of lithium atoms on liquid lithium surfaces has been done
  - 0.3 and 2 eV incident energy
  - 45 degrees incident angle
  - 473 K and 723 K surface temperatures
- Major changes have been made to the code to better incorporate lithium
  - Enabling lithium runs to be integrated into the distributed computing system already in use for hydrocarbon modeling (giving ~10x speed-up)
  - Calculation of ion fraction of reflected/sputtered atoms now built in
  - New liquid lithium potential data included†
- Currently running 543 K, 20-degree cases

†L.E.Gonzalez, private communication (2002).

PLASMA MATERIAL INTERACTION GROUP

Ionization probability of ejected alkali atoms at low energy





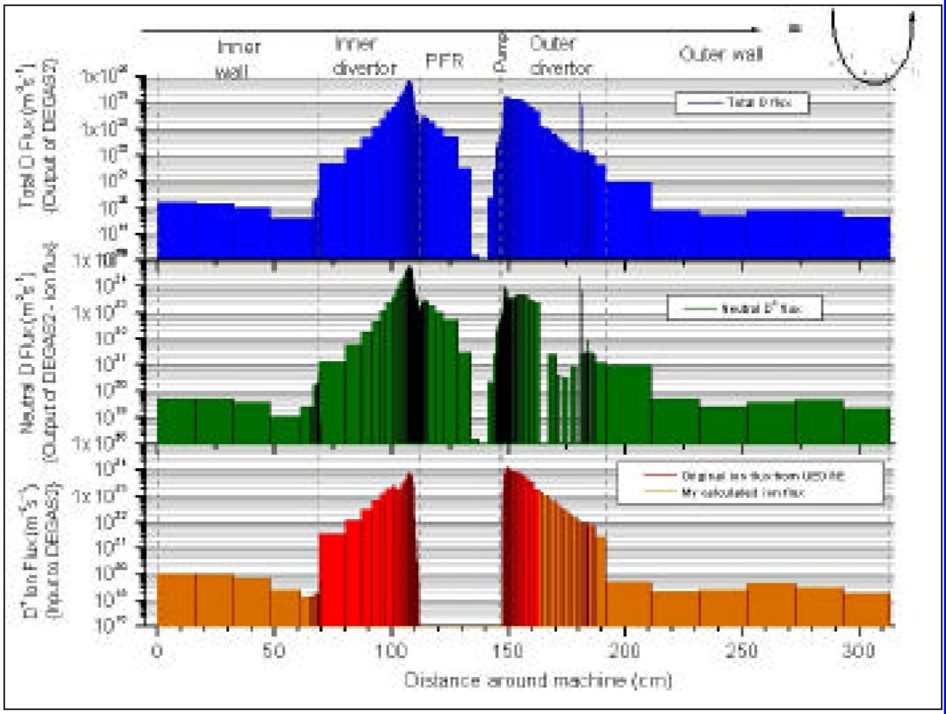
- The ionization probability has a strong dependence on outgoing velocity and surface work function (which depends on the surface thermodynamic and chemical state).
- At lower outgoing velocities and oblique emissions, alkali backscattered and backsputtered atoms are neutralized near the surface.
- For liquid lithium without any adsorbates or oxides the average surface work function is 2.9 eV[1]. For the case of 0.35 eV incident Li^+ at 20-degree incidence, the average backscattered energy is 0.25 eV with an average elevation angle of 15 degrees.

1. N.W. Aschcroft and N.D. Mermin, Solid State Physics, 1976, Saunders College Publishing

PLASMA MATERIAL INTERACTION GROUP

FIRE Be/W mixed material analysis

- Included fueling sources in DEGAS2 modeling
  - 100 torr/l-s pellet injection
  - 100 torr/l-s gas puffing
- Be sputtering source from first wall is $8.9\times10^{19}\ s^{-1}$
- WBC+ analysis shows Be currents of
  - $4.1\times10^{19}\ s^{-1}$ to inner divertor
  - $9.8\times10^{18}\ s^{-1}$ to outer divertor



- Be sputtering remains low - determining whether any part of the model needs refinement

HEIGHTS Results on ELMS

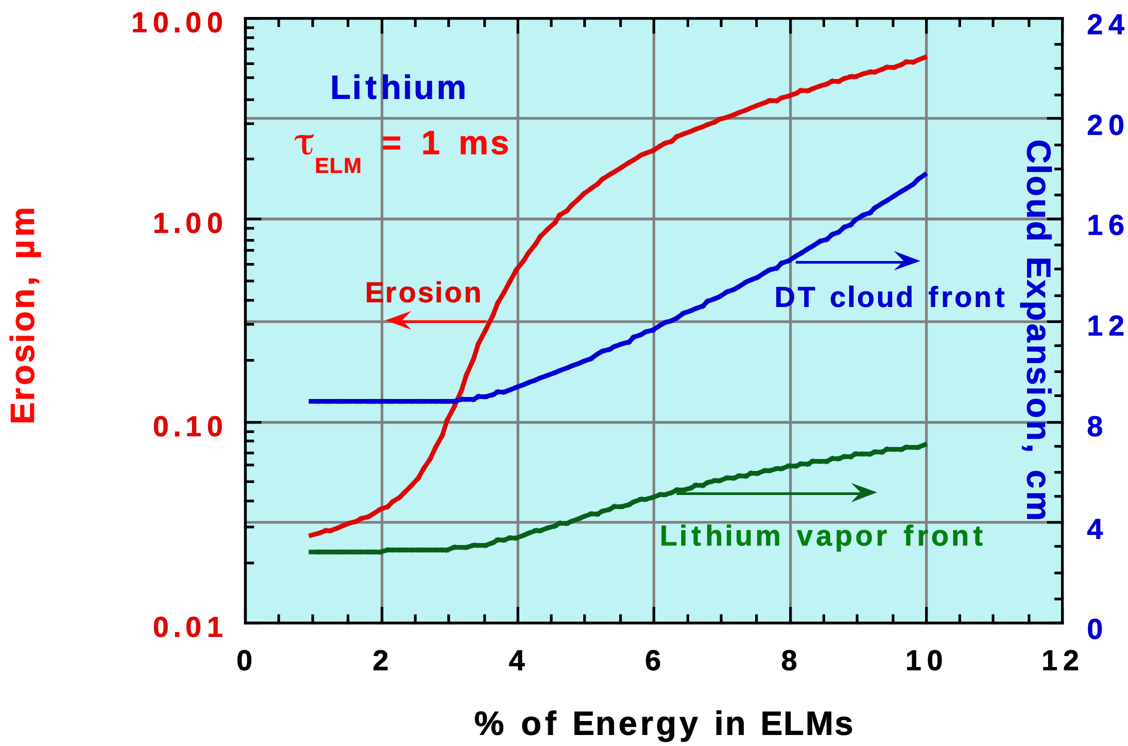
- **ELMs can be a serious concern for plasma-facing components during normal operation of next generation tokamaks. Unlike disruptions, we must be able to tolerate ELMs**

- **Two-fluid model is developed to integrate SOL parameters during ELMs with divertor surface evolution using HEIGHTS numerical simulation package. Liquid and solid materials being analyzed, for NSTX, ITER-type reactors, etc.**

- **HEIGHTS analysis indicates that there exist an ELM power *threshold* for each divertor material at which the periodic pulses of energy cause excessive target erosion and large vapor expansion.**

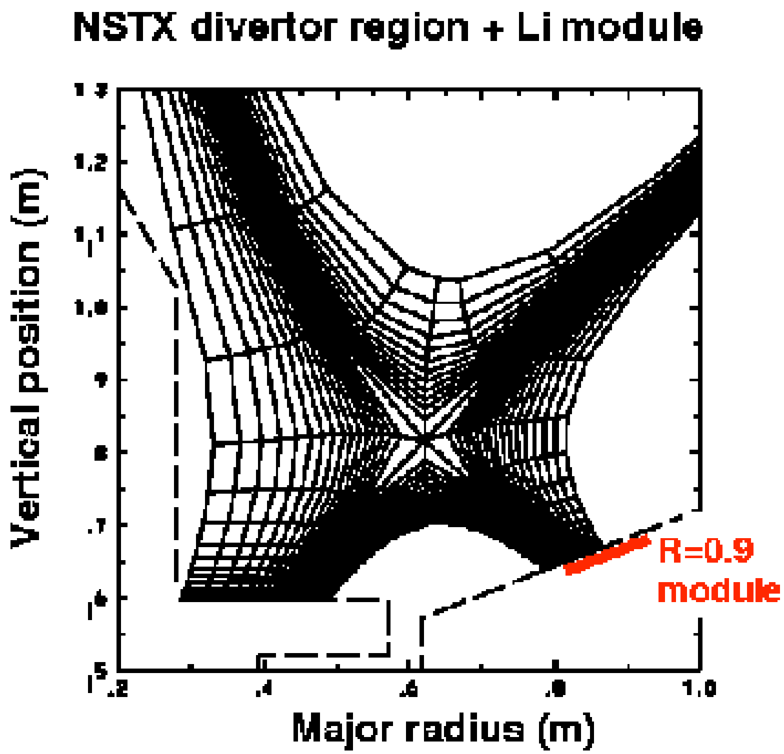
- **Large vapor expansion leads to plasma contamination and possible termination in a disruption even in renewable surface materials such as lithium where erosion is not a problem.**

HEIGHTS Calculations of Material Erosion and Cloud Expansion during ELMs



Lithium contamination of core from NSTX module modeled by coupling UEDGE & WBC

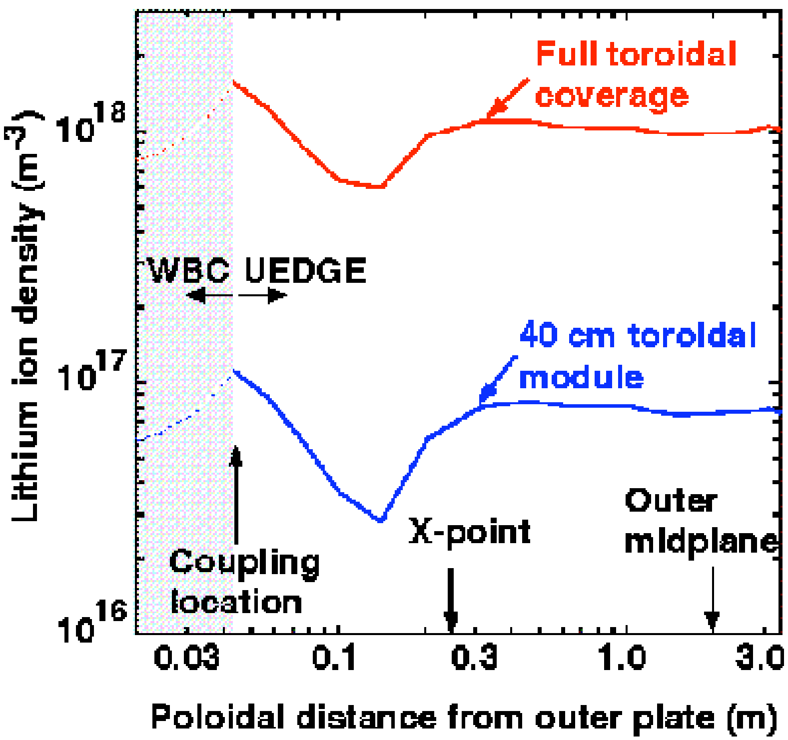
- **Heat and particle flux to module computed by UEDGE**
- **Temperature rise of Li surface from Ulrickson's model**
- **Sputtering of Li from U. Ill. composite model**
- **WBC calculates lithium source near the divertor plate**
- **UEDGE uses this Li source to calculate lithium density at core boundary**



Core-edge lithium concentration from 40 cm module is ~0.2% for 6 MW case

- UEDGE takes lithium ion source from WBC 5 cm above the plate
- Full SOL hydrogen/lithium plasma is then evolved to steady state with hydrogen core-edge density 4×10^{19}
- For the planned 40 cm (toroidally) module, only 0.2% Li at core edge
- For full toroidal coverage with 13 times more module gives 2.5% Li
- Even for full coverage, Li SOL radiation is only 6.4×10^4 W, or 1% of core input power; thus, no need to iterate WBC/UEDGE here

Lithium density vs. distance from plate along flux surface 0.3 cm in SOL



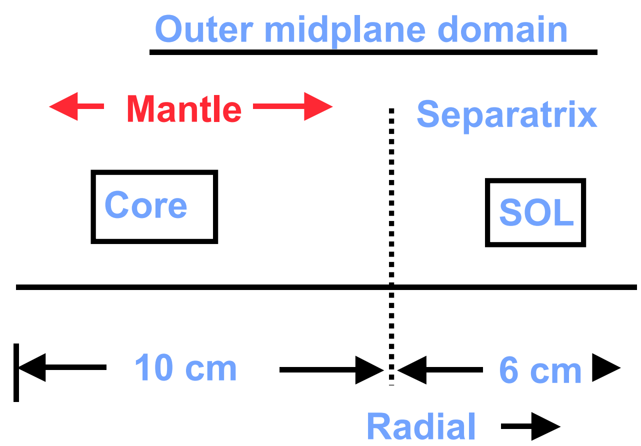
Large mantle impurity radiation is needed to give tolerable divertor heat loads even for liquids

The Problem:

- General issue for MFE devices; brought to the fore in CLIFF work
- 2-3 GW fusion power results in 400-600 MW of alpha power to remove
- UEDGE simulations give peak heat on orthog. divertor for SOL input:
  - 40 MW gives 27 MW/m^2
  - 80 MW gives 104 MW/m^2
  - 160 MW gives 186 MW/m^2
- Since heat flux needs < 50 MW/m^2, more than 80% of alpha power must be radiated

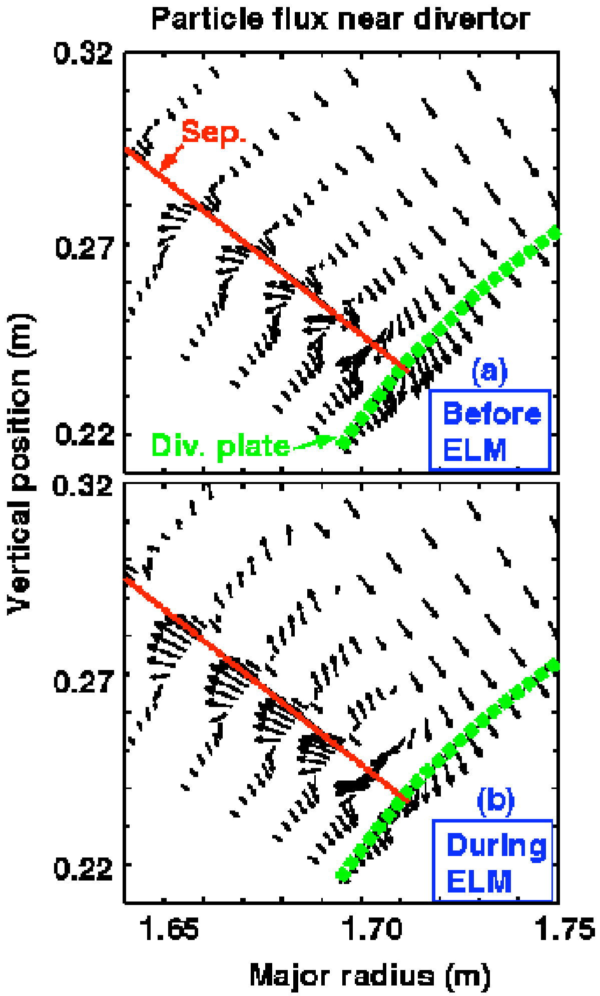
The approach:

- Extend UEDGE simulations to include mantle inside separatrix (expand from 1 cm to 10 cm)
- Investigate different impurities (Neon, Argon, Krypton)



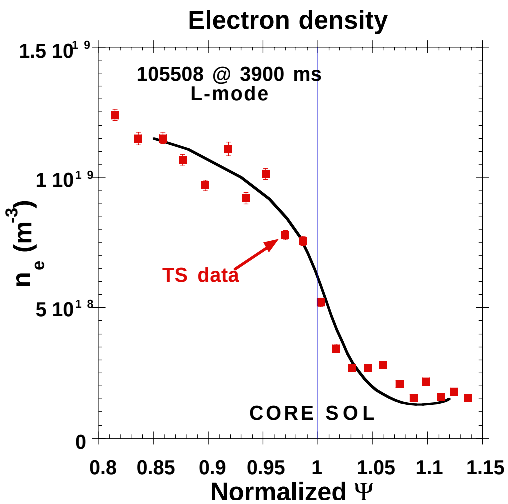
Time-dependent ELM modeling is being done by UEDGE

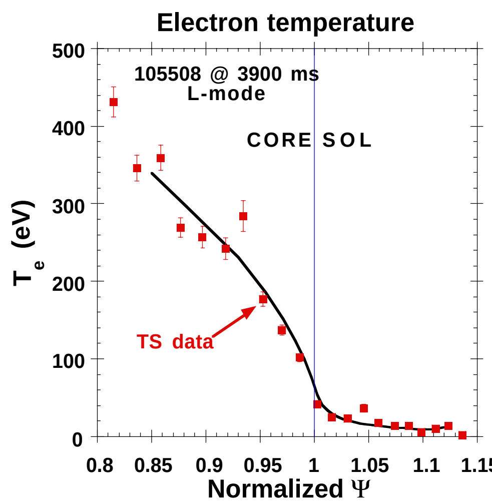
- UEDGE considers SOL currents and ExB drifts
- Characteristic two-time-scale seen: electron conduction and ion flow
- Parallel currents can dominate heat flow, causing outboard or inboard peaking, depending on current direction
- Can currents be manipulated to advantage?

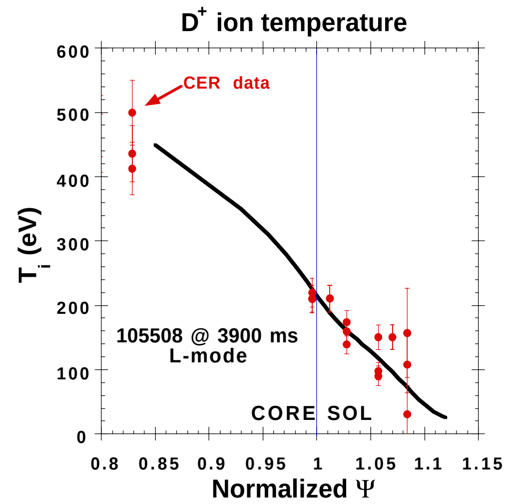


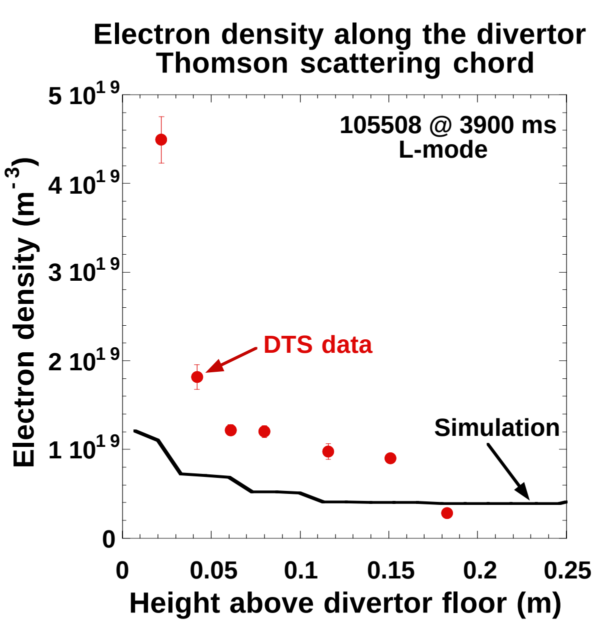
ExB drift causes strong reverse-flow near separatrix

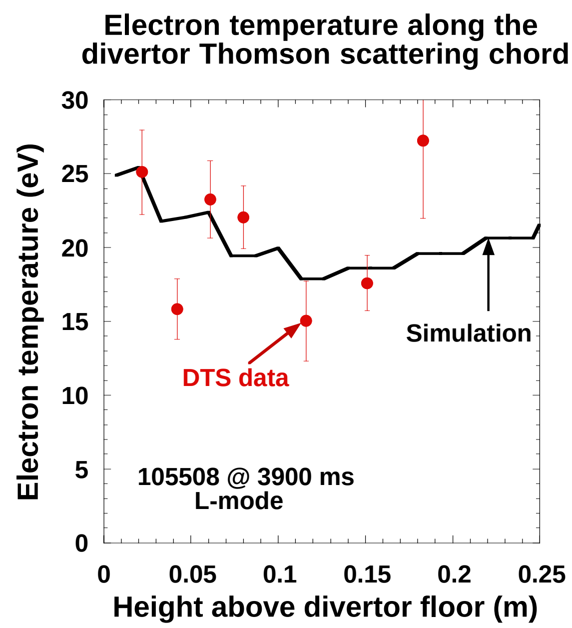
Background DIII-D DiMES Plasma Modeled and Supplied for Lithium Impurity Transport Analysis





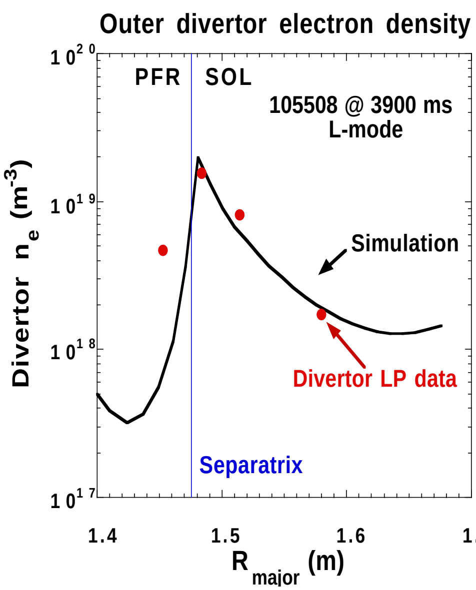


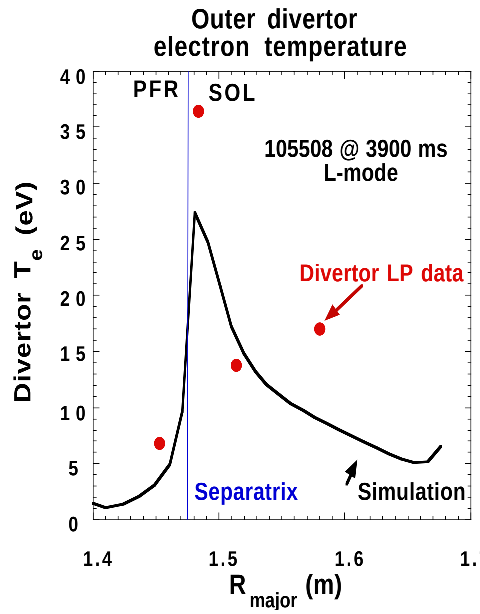


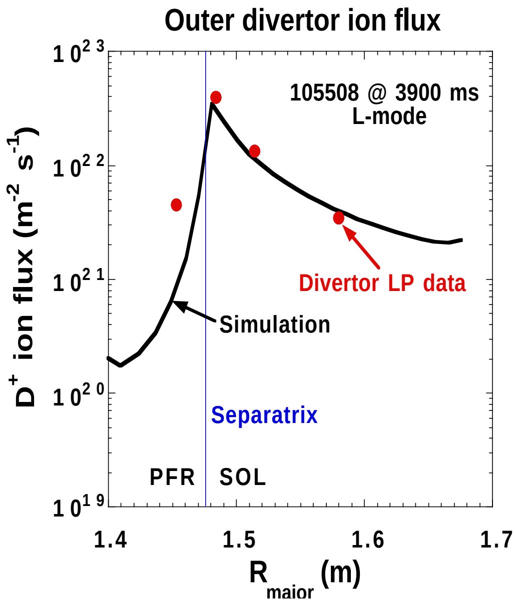


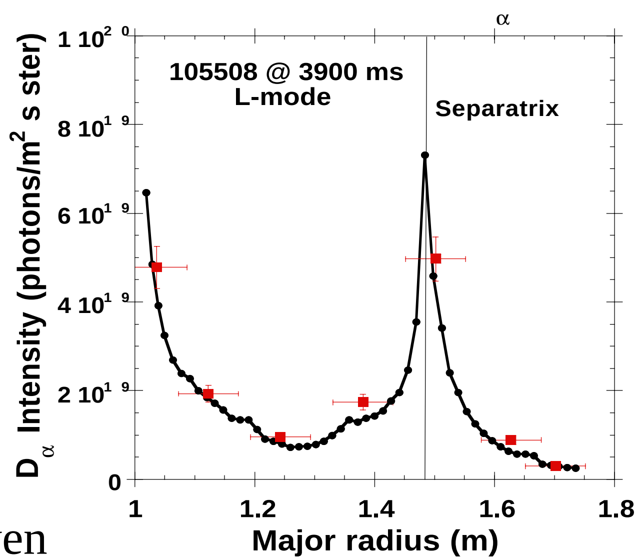
L. Owen

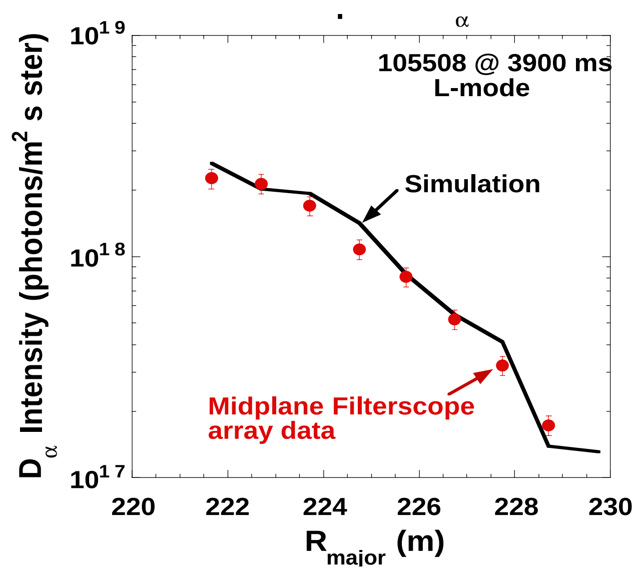
Background DIII-D DiMES Plasma Modeled and Supplied for Lithium Impurity Transport Analysis





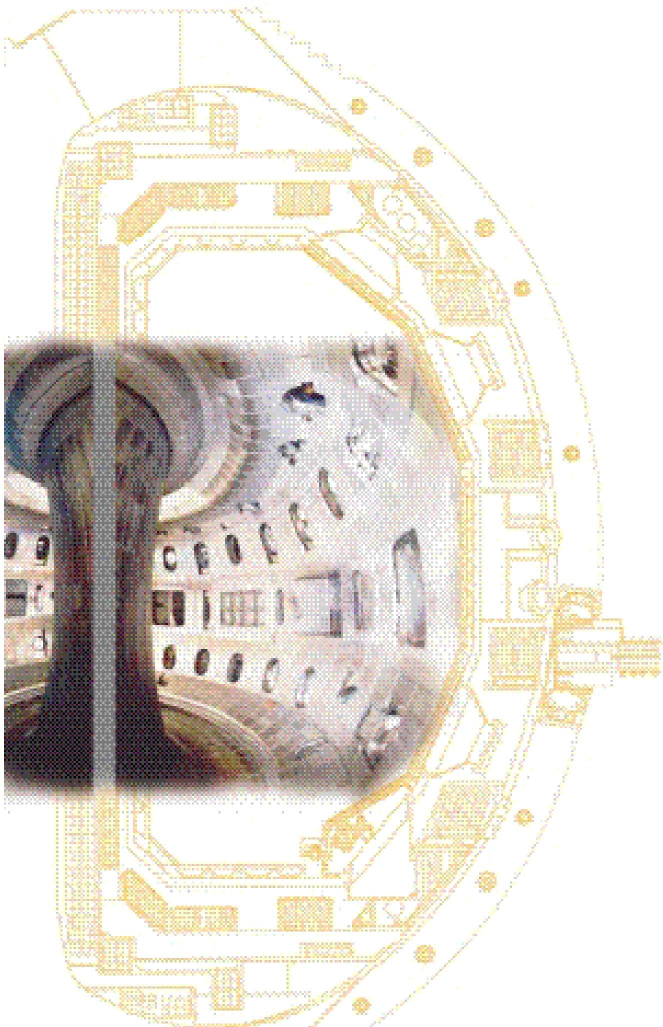






L. Owen

Lithium transport modeling in a low power DIII-D plasma



T. Evans[1], L. Owen[2], J. Brooks[3], D. Finkenthal[4], R. Maingi[2], D. Whyte[5], and C. Wong[1]

[1] General Atomics, San Diego, CA; [2] ORNL, Oak Ridge, TN; [3] ANL, Chicago, IL; [4] Palomar College, San Marcos CA; [5] University of Wisconsin, Madison, WI

ALPS/APEX Meeting

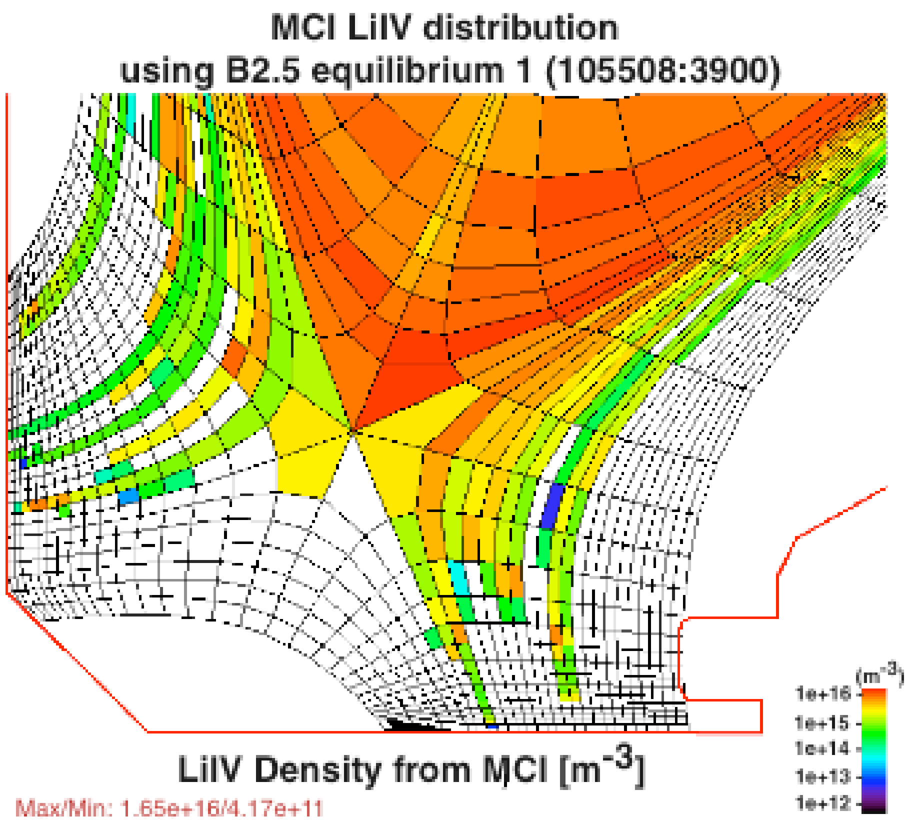
Wednesday 6 November 2002,

Princeton Plasma Physics Laboratory, Princeton New Jersey

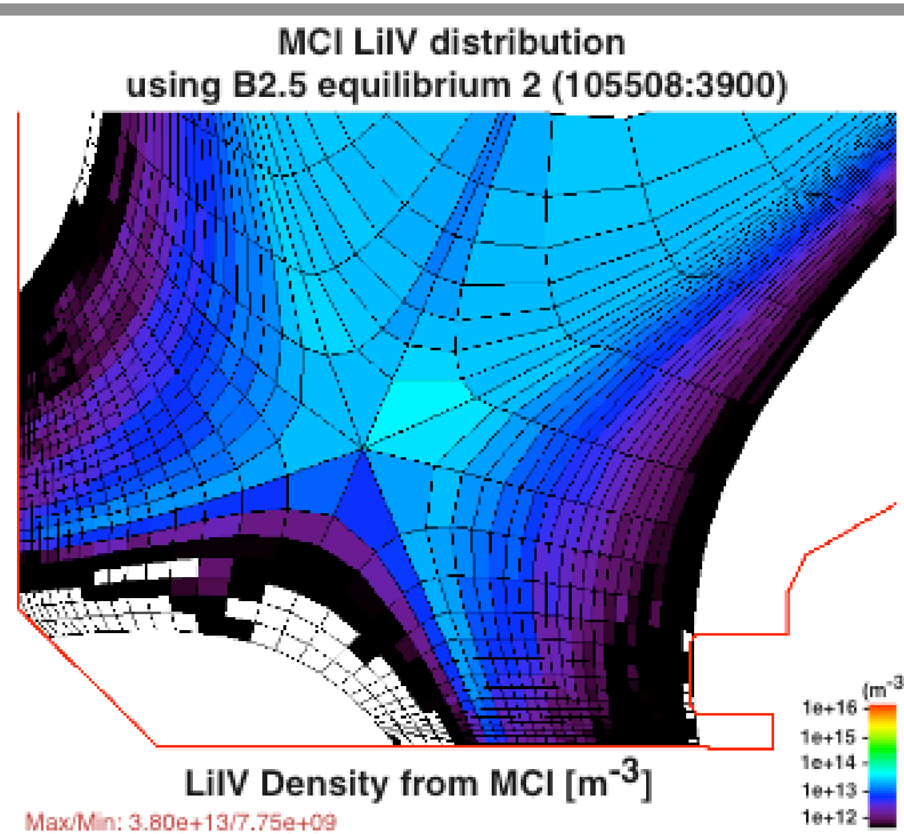
Lithium transport is being modeled in DIII-D with coupled fluid and kinetic codes

- Four specialized codes have been coupled to model Li sputtering and transport from a DIII-D DiMES sample
  - > background plasmas are simulated with the B2.5 / DEGAS fluid plasma / kinetic neutral deuterium code (L. Owen and R. Maingi at ORNL)
  - > Li sputtering sources are simulated with the gyro-kinetic WBC code (J. Brooks at ANL)
  - > Li transport is simulated by coupling the kinetic Monte Carlo Impurity (MCI) code to a B2.5 background plasma while using WBC Li sources (particle positions, velocities and charge states) as the initial conditions for the MCI simulation (T. Evans at GA and D. Finkenthal at Palomar)
- Simulations from the coupled codes will be compared to Li spectroscopic data from future DIII-D experiments where the edge Li concentration is increased to above 1% (the spectrometer resolution limit) by using very slow strike point sweeps across the Li sample.

The Li core concentration calculated in MCI is extremely sensitive to the B2.5 private flux region solution



$R_{div\text{-}in}$=0.925 & $R_{div\text{-}out}$ = 0.99
Core Li concentration ~ 0.1%



$R_{div\text{-}in}$= $R_{div\text{-}out}$ =1.0
Core Li concentration ~ 0.0002%

Suggests that drifts may need to be included in plasma model

DIII-D NATIONAL FUSION FACILITY SAN DIEGO

Summary

- B2.5 / DEGAS was successfully coupled to WBC and MCI in order to study Li transport during low power L-mode DIII-D Li DiMES experiments
- The sensitivity of the B2.5 private flux solutions, to boundary conditions such as divertor recycling, is a key Li impurity transport issue that needs to be resolved during future work.
- Preliminary Li transport results indicate a core concentration ranging between 0.0002% to 0.1% depending on T_e in the private flux region:
  - > These results are in agreement with experimental data indicating there is always less than 1% Li in the edge plasma during the discharge being simulated.
- Future work will focus comparing simulated LiIII edge radiation from MCI with spectroscopic LiIII data from DIII-D during very slow x-point sweeps (where edge LiIII concentrations will be forced to exceed 1%).

Neutral Gas Transport Simulations of Gas Puff Imaging Experiments

D. P. Stotler, B. LaBombard[2], R. J. Maqueda[1],
J. L. Terry[2], S. J. Zweben

Princeton Plasma Physics Laboratory
Princeton University
Princeton, NJ 08543

[1]Los Alamos National Laboratory
Los Alamos, NM 87545

[2]MIT Plasma Science and Fusion Center
Cambridge, MA 02139

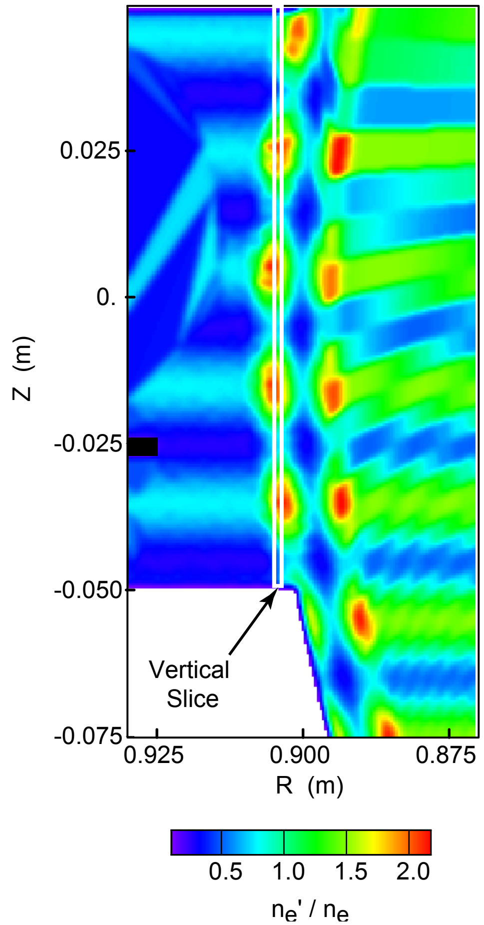
PRINCETON PLASMA PHYSICS LABORATORY

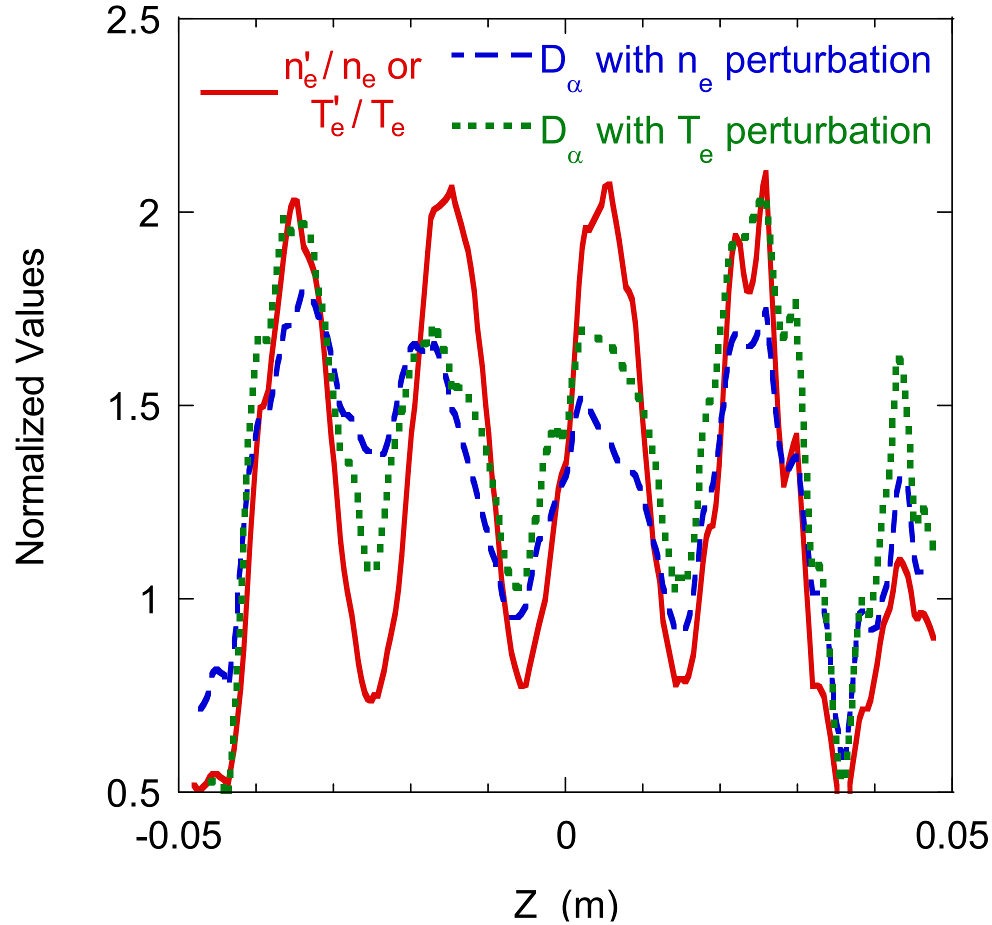
Gas Puff Imaging (GPI) Experiments Designed to Measure 2-D Structure of Edge Turbulence

- Puff neutral gas near outer wall,
- View with fast camera visible emission resulting from electron impact excitation of that gas,
- Use sightline $\parallel \vec{B}$ to see radial & poloidal structure.
  - Compare with turbulence measured by probes,
  - And with output from plasma turbulence codes.

Spatial Structure of Simulated Emission is Similar to That of Underlying Plasma Turbulence

⇒ Can at least qualitatively compare experimental wavenumber spectra with that from turbulence codes.





PPPL has developed a novel laser technique for removing tritium from plasma facing components.

This decade offers the prospect of construction of next-step DT burning tokamak(s) - FIRE, ITER, Ignitor

Arguably, the biggest technical risks in a burning plasma experiment are related to the choice of plasma facing components.

The public has a high sensitivity to tritium issues (witness closure of High Flux Beam Reactor at Brookhaven and National Tritium Labeling Facility at Berkley).

To date, there has been no tokamak scale demonstration of tritium removal - unlike any other aspect of a burning plasma experiment (e.g. remote handling).

We propose to demonstrate this technique at JET during the 2004 outage.

PPPL has developed a laser scanning detritiation technique. Lab experiments have removed up to 80% of tritium from tile samples from TFTR and JET (4 publications).

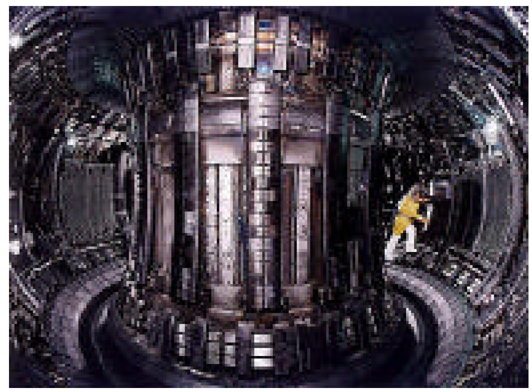
Method is attractive for a next step:

- Fiber optic coupling to in-vessel scanner
- Fast: estimated scan time ≈ 3 hours for 50m^2
- Tritium released by thermal desorption - no oxygen to decondition plasma facing surfaces or DTO exhaust to process.

JET provides a unique opportunity to prove this technique.

TFTR & JET tile samples used to date were exposed to air for extended periods - flaking and oxygen absorption may have changed thermal properties - In-vessel tests are essential.

Proposal also investigates in microscopic detail the critical topic of the interaction of high heat flux with tokamak generated materials - carbon codeposits as well ion damaged tungsten, berylium and mixed materials.



JET interior:
Only tokamak with DT capability.
Remote handling technology in place.

Proposal consistent with JET timetable:

- April 2002 - Define in-vessel activities for the 2004 shutdown
- Dec 2002 - Complete detailed design of in-vessel components
- Dec 2003 - End of Remote Handling trials
- Spring 2004 - In-vessel components to be ready for installation

Development work needed:

- Package present table top setup into module for carriage by remote manipulator arm.
- Electronics for remote control capability
- Qualifying trials at JET in CY 2003

Work supported by IAEA coordinated research plan on 'Tritium Inventory in Fusion Reactors"